## **Supplementary materials:**

## Electron Beam Induced Evolution in Au, Ag, and Interfaced Heterogeneous Au/Ag Nanoparticles

Yuzi Liu, Yugang Sun

Center for Nanoscale Materials, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States



**Figure S1.** Schematic illustrations highlighting the lattice planes of (a) (111) (labeled in cyan), (b) (001) (labeled in dark green), and (c) (101) (labeled in purple) in a 2x2x2 crystalline face-centered cubic (FCC) lattice. The ligth blue polyhedrons highlight the nearest neighboring vertex atoms (blue) of an atom (at the center of each polyhedron) in the FCC lattice.



**Figure S2.** 4 nearest neighbors (purple) of the atoms at the corner of (111), (11-1) and (1-10). Other 8 nearest neighbor (blue) missed. This sample just shows that the corner atoms lose more nearest neighbors.



**Figure S3.** A typical HREM image showing the sharp interfaces and crystalline epitaxy between the Ag and Au domains in each interfaced Au/Ag dimers.



**Figure S4.** EDX spectrum taken from the nanoparticle shown in Figure 6d with a nanobeam in TEM. The spectrum exhibits strong signals of Au while no Ag signals can be observed, indicating that the Ag atoms have been completely sublimated from the Au@Ag core@shell particles shown in Figure 6c.



**Figure S5.** Simulated differential cross section  $(d\sigma/d\Omega)$  as a function of scattering angle  $\Theta_{\perp}$ 



**Figure S6** Efficiency for energy transfer from the 200-KeV electrons to Au (black) and Ag (red) as a function of scattering angle  $\Theta$ . The dashed lines highlight whether the transferred energy can overcome the surface binding energy of Au (black) and Ag (red) to sublimate metal atoms.



**Figure S7.** Bright-field TEM images of Au nanoparticles before (a, c) and after (b, d) illumination of electron beams with different beam intensities: (a, b)  $1.5 \text{ pA/cm}^2$  and (c, d)  $7.5 \text{ pA/cm}^2$ .

## **Energy transfer from electron beam to atoms:**

The energy transfer from electrons to atoms is governed by momentum conservation. The scattering angle dependence of the energy T transferred to the nucleus is given by<sup>1</sup>

$$T(\Phi) = T_{max} \cos^2(\Phi) \tag{S1}$$

Figure S8 illustrates the geometry of electron scattered by atom nucleus. At the scenario of headon collision ( $\Phi$ =0), the transferred energy from electron to atom nucleus is maximum as <sup>1-4</sup>

$$E_{\max} = \frac{2M_A E_0 (E_0 + 2m_e c^2)}{(m_e + M_A)^2 c^2 + 2M_A E_0}$$
(S2)

Where  $M_A$  is the atom nucleus mass,  $m_e$  is the electron mass, c is Speed of light in vacuum,  $E_0$  is the electron beam energy.

It should be mentioned here, the electron must be treated as relativistic particle since its velocity is about 0.7c.

Because  $M_A/m_e=1823 Z >>1$  and  $E_0 << M_A c^2$ , where Z is the atomic mass number.

$$E_{\rm max} = \frac{2E_0(E_0 + 2m_ec^2)}{M_Ac^2}$$
(S3)

$$E_{\rm max} = \frac{E_0 (1.02 + E_0 / 10^6)}{465.7Z}$$
(S4)

From equation S3, we can see that the maximum transferred energy is only inversely proportional to its atomic mass number if the electron beam energy is constant. (in our experiment,  $E_0=200$ keV)



Figure S8 The diagram shows the scattering of electron by atom nucleus.

1. Vajda, P., Anisotropy of electron radiation damage in metal crystals. *Rev. Mod. Phys.* **1977**, *49* (3), 481-521.

2. Banhart, F., Irradiation effects in carbon nanostructures. *Rep. Prog. Phys.* **1999**, *62* (8), 1181.

3. Egerton, R. F.; McLeod, R.; Wang, F.; Malac, M., Basic questions related to electron-induced sputtering in the TEM. *Ultramicroscopy* **2010**, *110* (8), 991-997.

4. Egerton, R. F.; Li, P.; Malac, M., Radiation damage in the TEM and SEM. *Micron* **2004**, *35* (6), 399-409.